SHPECK - A GEOCHEMICAL EQUILIBRIUM SPECIATION MODEL

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ABSTRACT: Geochemical speciation is useful for calculating and modeling the distribution of dissolved solute and complex compound species in water, and also to compute saturation indices of minerals. In this work, we introduce SHPECK, a numerical method to calculate geochemical speciation using the mass-balance conditions and the phase rule. SHPECK uses the thermodynamic equilibrium reactions as equations for the calculation of multiphase systems in equilibrium. A set of mass-action equations aside with additional equilibrium constraints will compose the system and the number of species defines the number of equations necessary to solve the system. We apply the Newton-Raphson method to iteratively solve the system of nonlinear equations and converge to a solution. A geochemical speciation method is strongly related to the thermodynamic data used to represent the reactions. In SHPECK the information on elements, solutes, species, compounds, reactions details and equilibrium constants is collected from the Lawrence Livermore National Laboratory (LLNL) and organized in a SQL database. SHPECK's SQL database enables access to the thermodynamics through SQL queries, reducing the complexity and increasing the speed on information retrieval. We also implemented in SHPECK different approaches for calculating the activity coefficient: Davies, B-Dot and Debye - Huckel. To test and validate SHPECK we modeled the diagenetic reactions observed in Snorre Field reservoir sandstones of Norwegian North Sea. The main reservoir horizons of the field are the fluvial sandstones in the upper member of the Upper Triassic Lunde Formation and the Upper Triassic to Lower Jurassic Statfjord Formation. The sandstones are dominantly fine- to medium-grained and arkosic with framework constituents of quartz (40-80%), K-feldspar (5-12%), plagioclase (15-45%), muscovite, biotite and clay minerals. That includes smectite, mixed-layer clay minerals, chlorite and subordinate amounts of kaolinite and illite. Subordinate rock fragments include intraformational mudstone and carbonate clasts and extrabasinal grains of quartz-feldspar-mica aggregates that probably represent granitic rocks and/or schist or gneisses. The description of the diagenetic reactions that take place in the Snorre Field allowed us to generate results to carry out a computationally comparative study. We modeled the diagenetic processes that best represent the behavior of ions in the water-rock interactions using three models SHPECK, PHREEQC and MINTEQA2. The comparative study tested temperatures from 25 to 100 degrees Celsius with the same chemical composition of the seawater. The results of SHPECK are found to be consistent with the other commercially available geochemical equilibrium software tools. The accuracy of SHPECK is equivalent and within the expected range to the case study developed; the results were compared and, with the same input, they are nearly the same. Slight differences were found when simulating with temperatures higher that 100 degrees Celsius, which appear arise from discrepancies in how the thermodynamics properties are handled.

KEYWORDS: GEOCHEMICAL MODELING, WATER-ROCK INTERACTIONS, CHEMICAL EQUILIBRIUM SPECIATION.